

10/705,466

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* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 19:29:07 ON 14 NOV 2004

=> fil reg

COST IN U.S. DOLLARS

SINCE FILE
ENTRY

TOTAL
SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'REGISTRY' ENTERED AT 19:29:18 ON 14 NOV 2004
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STRUCTURE FILE UPDATES: 12 NOV 2004 HIGHEST RN 780001-49-2
DICTIONARY FILE UPDATES: 12 NOV 2004 HIGHEST RN 780001-49-2

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

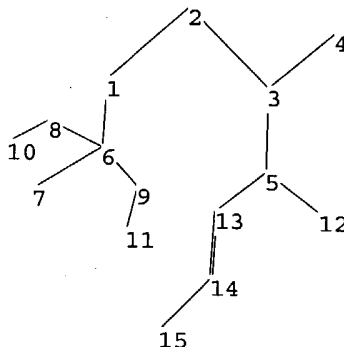
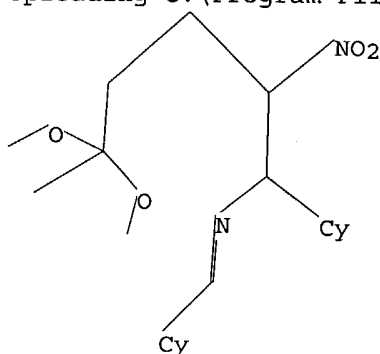
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Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
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=>

Uploading C:\Program Files\Stnexp\Queries\10705466.str



chain nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15

chain bonds :

1-2 1-6 2-3 3-4 3-5 5-12 5-13 6-7 6-8 6-9 8-10 9-11 13-14 14-15

exact/norm bonds :

5-12 5-13 6-8 6-9 8-10 9-11 13-14 14-15

exact bonds :

1-2 1-6 2-3 3-4 3-5 6-7

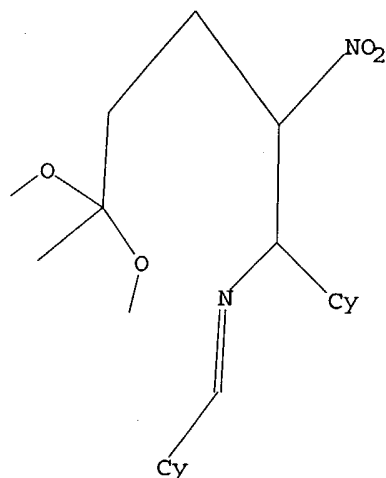
Match level :

1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS
10:CLASS 11:CLASS 12:Atom 13:CLASS 14:CLASS 15:Atom

L1 STRUCTURE UPLOADED

=> d query

L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1

SAMPLE SEARCH INITIATED 19:29:31 FILE 'REGISTRY'
 SAMPLE SCREEN SEARCH COMPLETED - 0 TO ITERATE

100.0% PROCESSED 0 ITERATIONS 0 ANSWERS
 SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
 BATCH **COMPLETE**
 PROJECTED ITERATIONS: 0 TO 0
 PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s l1 full

FULL SEARCH INITIATED 19:29:34 FILE 'REGISTRY'
 FULL SCREEN SEARCH COMPLETED - 2 TO ITERATE

100.0% PROCESSED 2 ITERATIONS 2 ANSWERS
 SEARCH TIME: 00.00.01

L3 2 SEA SSS FUL L1

=> fil caplus

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
155.42	155.63

FULL ESTIMATED COST

FILE 'CAPLUS' ENTERED AT 19:29:37 ON 14 NOV 2004

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FILE COVERS 1907 - 14 Nov 2004 VOL 141 ISS 21
FILE LAST UPDATED: 12 Nov 2004 (20041112/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l3

L4 2 L3

=> d l4 1-2 abs ibib hitstr

L4 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN
 AB This document discloses a process for preparing a pure cis isomer from a mixture of cis-trans isomers of formula $RC(OMe)2CH2CH2CH(NO2)CH(Ar)N:CHAr$ (I) [Ar = (un)substituted Ph, etc.; R = alkyl] comprising the steps of:
 (a) dispersing a mixture of cis- and trans-I in an inert solvent wherein said cis isomer is less soluble than said trans isomer; (b) heating said dispersion to completely dissolve said trans isomer; (c) maintaining said heating step to allow interconversion of said cis and trans isomer; (d) cooling said mixture thereby crystallizing the cis isomer; (e) separating said crystalline cis isomer from said solvent. Cis isomers of formula I are useful intermediates in the synthesis of cis isomers of benzamide piperidine compds. which exhibit activity as NK-1 receptor antagonists.

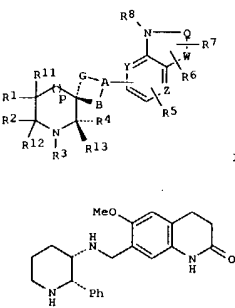
ACCESSION NUMBER: 2004:428898 CAPLUS
 DOCUMENT NUMBER: 141:6912
 TITLE: Process for converting a cis-trans mixture of substituted benzylidene amines into the pure cis isomer
 INVENTOR(S): Humphrey, John Michael; Tom, Norma Jacqueline
 PATENT ASSIGNEE(S): Pfizer Products Inc., USA
 SOURCE: PCT Int. Appl., 21 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004043908	A1	20040527	WO 2003-1B4953	20031103
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
PRIORITY APPLN. INFO.: US 2002-425946P P 20021112				

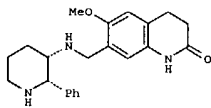
OTHER SOURCE(S): CASREACT 141:6912; MARPAT 141:6912
 IT 695165-42-5P
 RL: PUR (Purification or recovery); SPN (Synthetic preparation); PREP (Preparation)
 (process for converting a cis-trans mixture of substituted benzylidene amines into the pure cis isomer)
 RN 695165-42-5 CAPLUS
 CN Benzenemethanamine, α -(4,4-dimethoxy-1-nitrohexyl)-N- (phenylmethylene)-, [N(2)]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

L4 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN
 GI



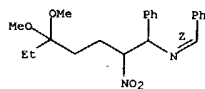
I



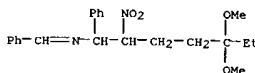
II

AB Title compds. I [Q = C:NH, C:CH2, C:S, C:O, SO, SO2; A = CH, CH2, C(alkyl), CH(alkyl), C(CF3), or CH(CF3) with the proviso that when B is present, A = CH, C(alkyl), or C(CF3); B = absent, CH2, or ethylene; Y, Z = N, CH, provided that both are not N; G = NH(CH2)q, S(CH2)q, O(CH2)q; q = 0-1 with the proviso that when q = 0, G = NH2, SH, OH; W = 1-3 carbon linking group, including spiro assemblies; p = 0-2; R3 = H, acyl, carboxy, Ph, heterocyclyl, alkyl, etc.; R1, R2, R11-13 = H, alkyl, etc., or R12-13 together with the carbon atoms to which they are attached form a 5- or 6-membered heterocyclic ring, etc.; R4 = Ph, pyridyl, thienyl, etc.; R5-8 = H, alkyl, S(O)1-2-alkyl, S(O)1-2-aryl, alkoxy, halo, Ph, etc.] were prepared. Approx. 100 synthetic examples and over 100 precursor preps. were provided. For instance, 4-aminophenol was acylated with 3-chloropropionyl chloride (CH2Cl2, H2O, NaHCO3, room temperature, 4 h) and the product treated with AlCl3 at 210°C for 10 min effecting cyclization to the hydroxy quinoline intermediate. The intermediate was O-methylated (acetone, Me2SO4, K2CO3, room temperature, 16 h) and formulated in the 7 position (CH2Cl2, AlCl3, Cl2CHOMe) to give 7-formyl-6-methoxy-1H-1,2,3,4-tetrahydroquinolin-2-one. Reductive alkylation of the quinolone with (2S,3S)-3-amino-2-phenylpiperidine (a. PhMe, 3A mol. sieves; b. dichloroethane, NaBH(OAc)3, room temperature, 16 h) yielded II. Compds. I are NK-1 receptor antagonists, i.e., substance P receptor antagonists. At least one

L4 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



IT 368935-48-7P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (process for converting a cis-trans mixture of substituted benzylidene amines into the pure cis isomer)
 RN 368935-48-7 CAPLUS
 CN Benzenemethanamine, α -(4,4-dimethoxy-1-nitrohexyl)-N- (phenylmethylene)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
 FORMAT

L4 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
 stereoisomer of the example compds. had a binding affinity, as measured by

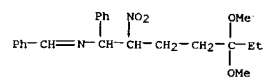
K1, of at least 600 nM. I are used in the treatment and prevention of a wide variety of central nervous system disorders, inflammatory disorders, cardiovascular disorders, ophthalmic disorders, etc.

ACCESSION NUMBER: 2001:762988 CAPLUS
 DOCUMENT NUMBER: 135:331346
 TITLE: Synthesis of benzoamide piperidine containing compounds as substance P antagonists
 INVENTOR(S): Arnold, Eric Platt; Chappie, Thomas Allen; Huang, Jianhua; Humphrey, John Michael; Nagel, Arthur Adam; O'Neill, Brian Thomas; Sobolov-Jaynes, Susan Beth; Vincent, Lawrence Albert
 PATENT ASSIGNEE(S): Pfizer Products Inc., USA
 SOURCE: PCT Int. Appl., 209 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001077100	A2	20011018	WO 2001-1B629	20010406
WO 2001077100	A3	20020307		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SI, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG US 2003087925 A1 20030508 US 2001-811218 20010316 EP 1272484 A2 20030308 EP 2001-919702 20010406 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR BR 2001009936 A 20030506 BR 2001-9936 20010406 JP 2004501072 T2 20040115 JP 2001-575573 20010406 EE 200200588 A 20040415 EE 2002-588 20010406 NZ 521346 A 20040730 NZ 2001-521346 20010406 BG 107135 A 20030630 BG 2002-107135 20020923 ZA 2002008072 A 20031008 ZA 2002-8072 20021008 NO 2002004874 A 20021118 NO 2002-4874 20021009 PRIORITY APPLN. INFO.: US 2000-195922P P 20000410 US 2000-212922P P 20000620 WO 2001-1B629 W 20010406				

OTHER SOURCE(S): MARPAT 135:331346
 IT 368935-48-7P, Benzylidene-(5,5-dimethoxy-2-nitro-1-phenylheptyl)amine
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (intermediate; synthesis of benzoamide piperidine containing compds. as substance P antagonists)

L4 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
 RN 368835-48-7 CAPLUS
 CN Benzenemethanamine, α -(4,4-dimethoxy-1-nitrohexyl)-N-(phenylmethylene)- (9CI) (CA INDEX NAME)



=> logoff y
COST IN U.S. DOLLARS

FULL ESTIMATED COST

SINCE FILE	TOTAL
ENTRY	SESSION
11.28	166.91

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

CA SUBSCRIBER PRICE

SINCE FILE	TOTAL
ENTRY	SESSION
-1.40	-1.40

STN INTERNATIONAL LOGOFF AT 19:31:47 ON 14 NOV 2004